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Our aim in this period has been to devise a simple, physically intuitive model to study the quantitative trends of hot-electron behavior in semiconductor alloys. This is being done to offer preliminary guidance to experimental programs, and to serve as a simple limit to check the more elaborate calculations still to come. Even our simple model is based on fairly complete alloy band structures, and therefore constitutes an advance over previously published results.

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SEMICONDUCTOR ENGINEERING FOR HIGH-SPEED DEVICES

Quarterly R&D Status Report 2

Covering the Period 16 September to 15 December 1985

15 December 1985

By: A. Sher [Principal Investigator, (415) 859-4466]
S. Krishnamurthy, and A.-B. Chen
Physical Electronics Laboratory

Prepared for:

Air Force Office of Scientific Research
Bolling Air Force Base, D.C. 20332-6448

Advanced Research Projects Agency (DoD)
1400 Wilson Boulevard
Arlington, Virginia 22209

Attn: Captain Kevin Malloy, Program Manager
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SRI International®
333 Ravenswood Ave. • Menlo Park, CA 94025
(415) 326-6200 • TWX: 910-373-2046 • Telex: 334-486

I DESCRIPTION OF PROGRESS

This report summarizes major accomplishments during the period 16 September to 15 December 1985.

Our aim in this period has been to devise a simple, physically intuitive model to study the qualitative trends of hot-electron behavior in semiconductor alloys. This is being done to offer preliminary guidance to experimental programs, and to serve as a simple limit to check the more elaborate calculations still to come. Even our simple model is based on fairly complete alloy band structures, and therefore constitutes an advance over previously published results.

A. Approach

An appropriate model for a bulk semiconductor is described in Sze's book, Physics of Semiconductor Devices. We have generalized this model so it applies to alloys. The model assumes that the conduction electrons are in steady-state with a temperature T_e, that is different from the lattice temperature T. When two valleys are involved in hot-electron transport, as in the case of GaAs, the steady-state current density is given by

$$J = e(n_1\mu_1 + n_2\mu_2)\mathcal{E} = env \quad , \tag{1}$$

where $n_i\mu_i$ are respectively the concentration and low-field mobility in the i^{th} valley. Because the effective mass is very large for the higher valley, we have $\mu_2 << \mu_1$. Thus, Eq. (1) reduces to

$$v = \frac{\mu_1 \mathcal{E}}{(1+n_2/n_1)} \tag{2}$$

The use of this approximation limits the accuracy of the results on the high- field side of the velocity/field peak; however, the peak amplitude and position are given well. The electron temperature is determined from the energy balance equation.

$$e\mathcal{E}v = [\langle E(T_e)\rangle - \langle E(T)\rangle]/\tau_e \tag{3}$$

$$= \frac{3}{2} k (T_e - T)/\tau_e \quad ,$$

where < > indicates a thermal average and τ_e is the electron-lattice energy relaxation time. As a *first approximation*, τ_e is assumed to be 10^{-12} s. (Future detailed studies of hot-electron behavior will involve explicit evaluation of τ_e.) From Eqs. (2) and (3), we get

$$T_e = T + \frac{2e\tau_e}{3k} \mu_1 \mathcal{E}^2 \left[1 + \frac{n_2}{n_1}\right]^{-1} \tag{4}$$

$$v = \mu_1 \mathcal{E} \left[1 + \frac{n_2}{n_1}\right]^{-1} \quad . \tag{5}$$

Note that because n_2/n_1 depends on T_e, Eq. (4) must be solved self-consistently for T_e. Velocity field characteristics are then obtained from Eq. (5).

In the case of alloys, the alloy-scattering contribution to the electron mobility, μ_1, is calculated by using a generalized Brook's formula, developed by us previously. Standard results are used for acoustic and optical phonon scattering. We further generalized Eqs. (4) and (5) by treating μ_1 as a function of T_e. This is particularly necessary in semiconductor alloys. Because the energy difference between the satellite-minima and the lower central valley minima can be a decreasing function of alloy concentration, μ_1 will be affected considerably for larger T_e. For more accurate velocity-field characteristics, T_e was solved self-consistently, assuming that μ_1 and n_2/n_1 depend on T_e. Ultimately we plan to calculate the actual electron state population distributions, and will not assume the existence of an electron temperature, at which point n_1 and n_2 will have to be solved self-consistently.

B. Results

Figure 1 shows the fundamental gap (E_g), the energy difference between the L-minimum and the Γ-minimum of the lowest-lying conduction band (ΔE), and the peak velocity (v_p), plotted as a function of x for lattice

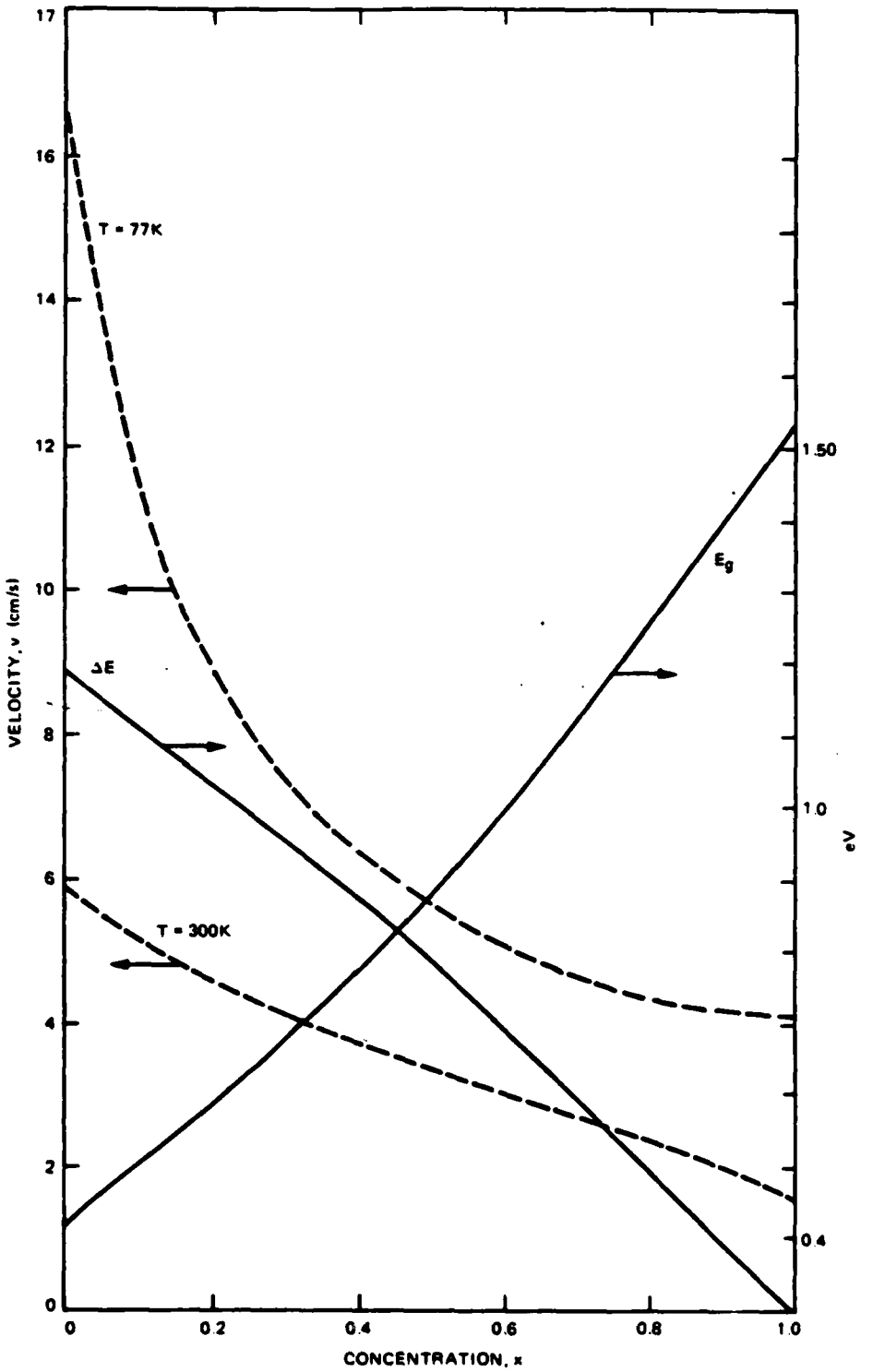

FIGURE 1 $Ga_xIN_{1-x}As$ COMPOSITION VARIATION OF PEAK DRIFT VELOCITY v_p AT 300K AND 77K (DASHED CURVES), ENERGY SEPARATION ΔE BETWEEN CONDUCTION BAND EDGE AND MINIMUM OF SATELLITE VALLEY, AND BAND GAP, E_g

temperatures T = 300K and 77K. We see that v_p can be increased by decreasing the GaAs concentration. However, E_g must be greater than ΔE to avoid avalanche breakdown.

The effect of breakdown is not explicitly included in the velocity/field calculations, and our results cease to be meaningful once the electrons gain sufficient energy to initiate breakdown. Hence, we conclude that the peak drift velocity v_p attains a realistic maximum as a function of alloy composition for x = 0.47 at T = 300K of 3.5×10^7 cm/s, which is about two times larger than that for GaAs. Experiments suggest a factor between 1.5 and 2.0. For a given concentration, v_p increases as T is lowered. Room-temperature velocity/field characteristics are given in Figure 2 for various values of x. (Remember that these curves are unrealistic for x > 0.47 where ΔE is less than E_g.) We see that $\mathcal{E}_{max}$, the field at which the velocity reaches a maximum, first increases with x and then decreases to the GaAs value. This trend is not seen in experiments. Figure 3 shows room-temperature velocity/field characteristics for very high fields. Notice that despite the use of Eq. (2), the high field v still increases with $\mathcal{E}$ for pure GaAs (x = 1). Just above the peak, v for alloys with x < 1 are higher than that for x = 1 (GaAs). The trend is reversed at still higher fields (~100 kV). The "crossover" takes place between x = 0.47 and x = 1 curves near $v = 1 \times 10^7$ cm/s. This phenomena has been confirmed by experiment. However, the calculated $\mathcal{E}$ at which the crossover takes place is much larger than the experimental value of 25 kV/m. The discrepancies mentioned above are due mostly to the assumed constancy of the τ_e and the approximation leading to Eq. 2. However, truly quantitative results must await the more elaborate calculations we have planned.

One needs the molecular coherent potential approximation (MCPA) self energies to properly calculate the alloy-scattering contributions to the electron mobilities used to obtain the results described earlier. In the calculation of the low-field mobility, only the self energies near the conduction band edge are needed. In this preliminary result, the MCPA self-energy matrix is expanded in terms of the averaged scattering T-matrix. By considering only the first two terms in the expansions, we have shown that the resulting self-energies near the band-edge are in excellent agreement

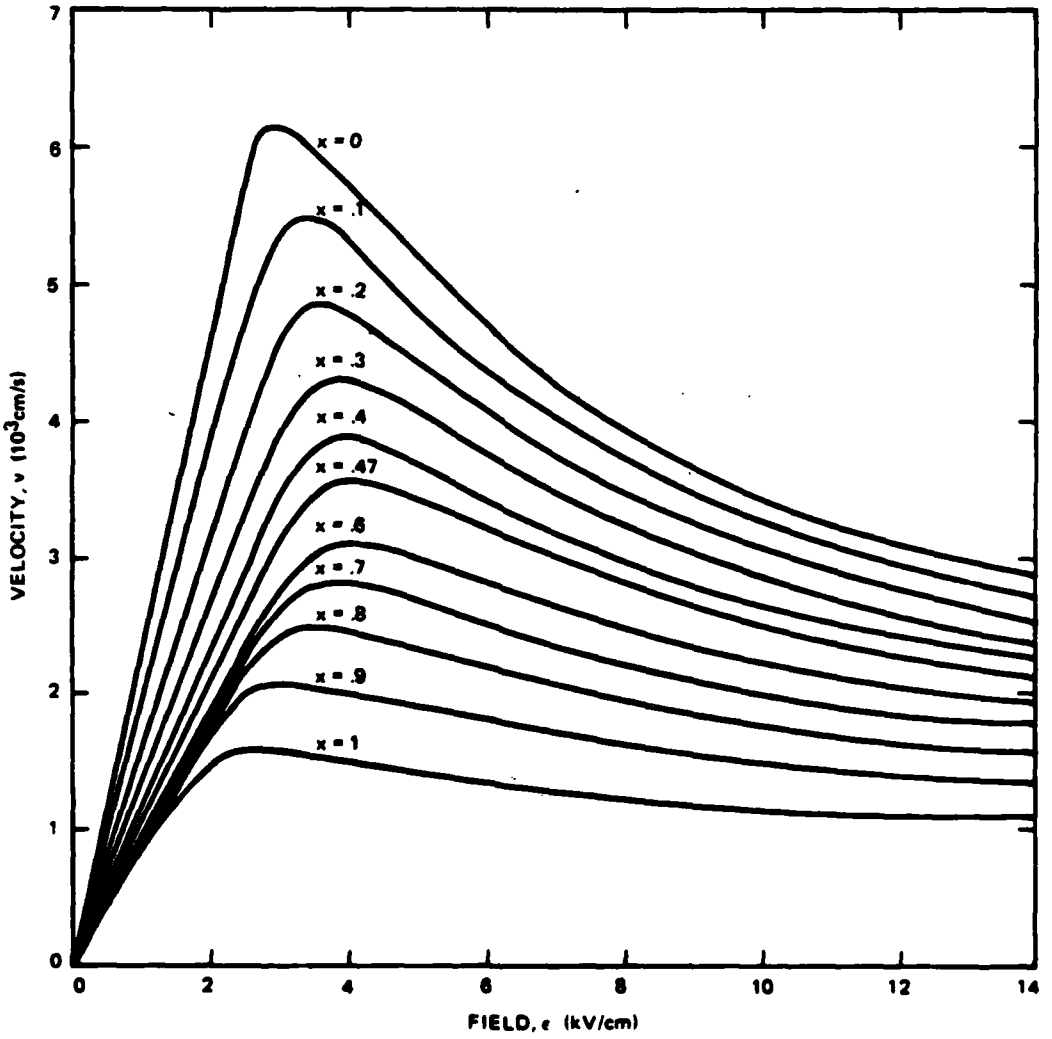

FIGURE 2 VELOCITY/FIELD CHARACTERISTICS OF $Ga_xIn_{1-x}As$ ALLOYS FOR DIFFERENT CONCENTRATIONS OF x AT T = 300K

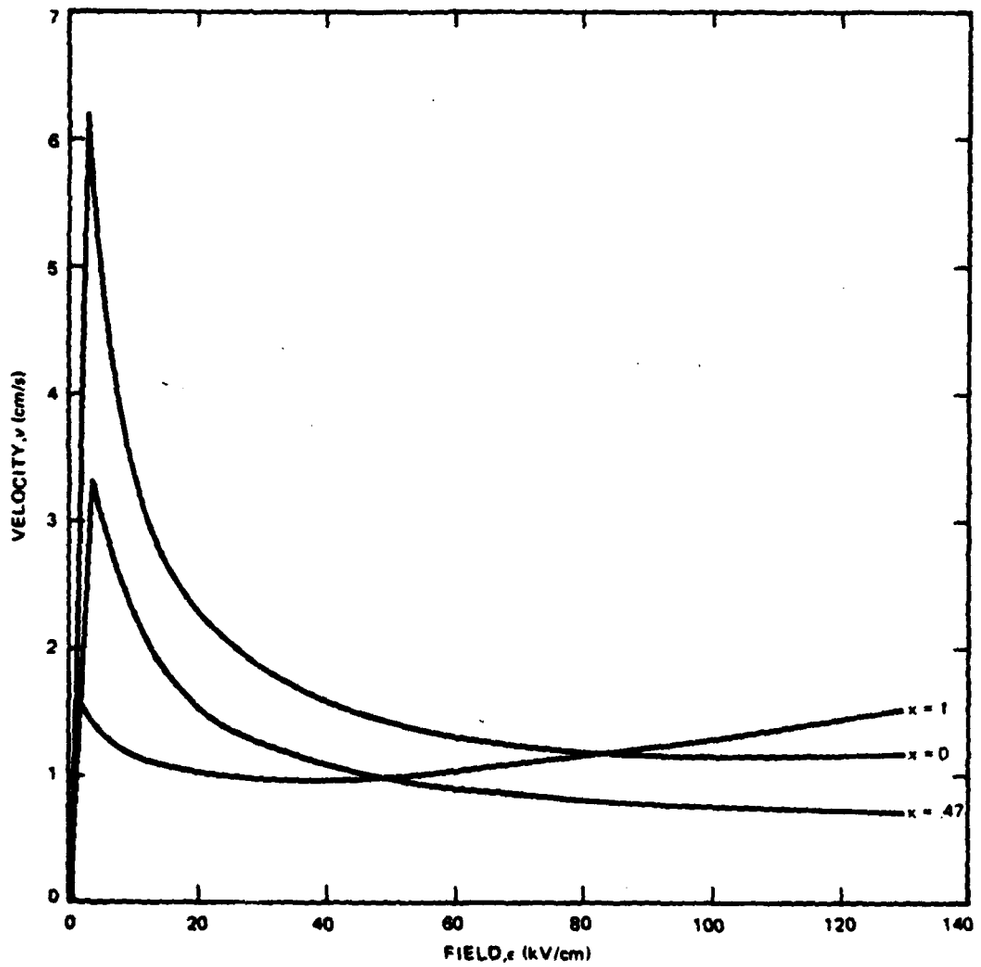

FIGURE 3 VELOCITY/FIELD CHARACTERISTICS OF $Ga_xIn_{1-x}As$ ALLOYS FOR DIFFERENT CONCENTRATIONS OF x AT T = 300K – HIGH-FIELD CASE

with the ones obtained from a rigorous MCPA calculation. For energies 1.0 to 1.5 eV from the band edge, an accuracy of about 90 percent could be achieved. Because this procedure entails a perturbative expansion, MCPA self energies could be calculated without inversion of 16 x 16 matrices for every $\vec{k}$ in the Brillouin zone. The procedure and results of these calculations are being written for publication in Applied Physics Letters. However, this approximation will be removed once our CRAY time becomes available.

II EQUIPMENT PURCHASED OR CONSTRUCTED

None.

III TRIPS, MEETINGS, PAPERS, AND VISITS

Three papers have been submitted to the March APS Meeting:

- "Preliminary CPA Velocity-Field Characteristics of Semiconductor Alloys," S. Krishnamurthy, A.-B. Chen, and A. Sher.
- "Calculation of Band-Edge Properties of Semiconductor Alloys," A. Sher, S. Krishnamurthy, Y.-M. Lai Shih, and A.-B. Chen.
- "Electronic Properties of HgZnTe," M. Berding, S. Krishnamurthy, A. Sher, and A.-B. Chen.

These papers also will be written for publication.

IV PROBLEMS OR AREAS OF CONCERN

We have requested extra computer time, and time on a CRAY is being arranged.

V DEVIATION FROM PLANNED EFFORT

None.

VI FISCAL STATUS

The total contract funding for the three-year period is $611,296. Of this $195,287, is allocated to the first year. Including the burden, approximately $22,000 is intended to pay the consulting fee of An-Ban Chen

leaving approximately $173,000. In the first two quarters ending 7 December 1985, we spent approximately $86,500, leaving $86,500 for the remaining two quarters, ending 31 May 1986. Thus, our expenditure rate is on schedule.